

The role of diffusion in branching and annihilation random walk models

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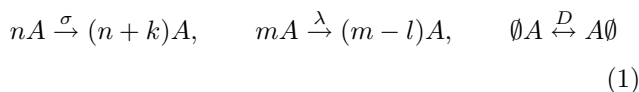
Different branching and annihilating random walk models are investigated by cluster mean-field method and simulations in one and two dimensions. In case of the $A \rightarrow 2A$, $2A \rightarrow \emptyset$ model the cluster mean-field approximations show diffusion dependence in the phase diagram as was found recently by non-perturbative renormalization group method (L. Canet et al., cond-mat/0403423). The same type of survey for the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model results in a reentrant phase diagram, similar to that of $2A \rightarrow 3A$, $4A \rightarrow \emptyset$ model (G. Ódor, PRE **69**, 036112 (2004)). Simulations of the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model in one and two dimensions confirm the presence of both the directed percolation transitions at finite branching rates and the mean-field transition at zero branching rate. In two dimensions the directed percolation transition disappears for strong diffusion rates. These results disagree with the predictions of the perturbative renormalization group method.

I. INTRODUCTION

Phase transitions in nonequilibrium, dynamical systems, which do not satisfy the detailed balance condition and do not possess hermitian Hamiltonian may appear in models of population, epidemics, catalysis, cooperative transport [1], enzyme biology [2] and markets for example [3]. Many of the known systems can be mapped onto some reaction-diffusion models, the behavior of them are the studied intensively in the past decades [1,4]. In these systems particle (A) creation, annihilation and diffusion processes compete and by tuning the control parameters phase transition may occur from an active steady state to an inactive, absorbing state of zero density. The simplest example of such models exhibiting phase transition are the branching and annihilating random walk models (BARW), in which offsprings are created by a single ancestor: $A \rightarrow (n+1)A$ and particles annihilate: $2A \rightarrow \emptyset$.

The classification of universality classes of nonequilibrium systems is one of the most important tasks of statistical physics [5,6]. Universal scaling behavior may occur at continuous phase transitions like in equilibrium systems and the corresponding n -point correlations are homogeneous (but anisotropic) functions of space and time. In the past decades analytical and numerical studies explored a large zoo of such classes [6]. One may pose the important question: which are the relevant factors determining these classes? By inspecting the widespread literature it appears that besides the well known factors of homogeneous equilibrium models with short ranged interactions: i.e. spatial dimension, symmetries, conservation laws there are more things must be taken into account. For example due to the possibility of transitions in low dimensions topological effects may play important role [7]. Furthermore initial condition – as a boundary in the time direction – can also be relevant [8,9].

The mean-field classes of general,



site occupation number restricted models (with $n > 1$, $m > 1$, $k > 0$, $l > 0$ and $m-l \geq 0$) resulted in a series of different universality classes depending on n and m [10]. This means that above the upper critical dimension (d_c) of the transition n and m are relevant parameters. In particular for the $n = m$ symmetrical case the density of particles in the active phase, near the critical point ($\sigma_c > 0$) scales as

$$\rho \propto |\sigma - \sigma_c|^\beta, \quad (2)$$

with $\beta = 1$, while at the critical point it decays as

$$\rho \propto t^{-\alpha}, \quad (3)$$

with $\alpha = \beta/\nu_{||} = 1/n$ [11,10]. On the other hand for the $n < m$ asymmetric case continuous phase transitions at zero branching rate $\sigma_c = 0$ occur characterized by

$$\beta = 1/(m-n), \quad \alpha = 1/(m-1) \quad (4)$$

For $n > m$ the mean-field solution provides first order transition.

By going beyond the site mean-field approximation it turned out that the phase diagrams of the type eq.(1) models may contain other transition points with non-trivial scaling behavior. In previous papers [12,13] I investigated the $2A \rightarrow 3A$, $4A \rightarrow \emptyset$ model by cluster mean-field approximations and simulations in one and two dimensions and showed that the *diffusion* plays an important role: it introduces a different critical point besides the one obtained by site mean-field solution at $\sigma_c = 0$ (4). The non-trivial critical point at $\sigma_c > 0$, appearing by low diffusion rates exhibits the universal behavior of the transition of the $2A \rightarrow 3A$, $2A \rightarrow \emptyset$ (PCPD) model owing to the generation of the effective $2A \rightarrow \emptyset$ reaction via the quick processes: $2A \rightarrow 3A \rightarrow 4A \rightarrow \emptyset$ [14].

Very recent studies by Canet et al. [15,16] found similar diffusion dependence in the $A \rightarrow 2A$, $2A \rightarrow \emptyset$ BARW model. Using non-perturbative renormalization group

method (NPRG) they obtained a different phase diagram than what was expected by perturbative renormalization (RG) arguments [17]. Namely directed percolation (DP) transition were found in these models for $d > 2$ dimensions with $d_c = 4$. Furthermore those transitions at $\sigma_c > 0$ branching rate persist up to infinite dimensions provided λ/D is greater than a threshold value. This threshold value was found to be zero for $d < 3$ and finite for $d \geq 3$.

In this work I apply dynamical, cluster mean-field approximations for that BARW model and by extrapolations to $N \rightarrow \infty$ cluster sizes I determine the phase diagram in 1d. Furthermore I explore the phase transitions of the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model with this method and by simulations in one and two dimensions.

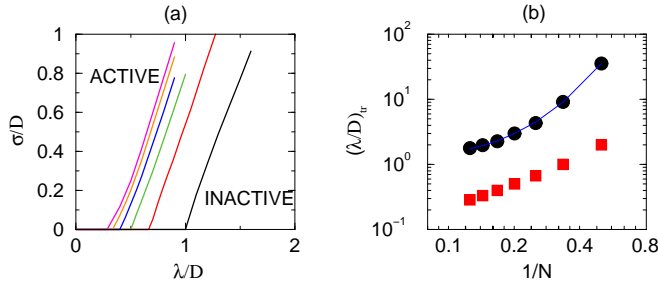


FIG. 1. (a) Phase diagram of the $A \rightarrow 2A$, $2A \rightarrow \emptyset$ model determined by $N = 3, 4, \dots, 8$ (right to left curves) cluster approximations. (b) The $(\lambda_c/D)_{tr}$ critical endpoint values of the $\sigma_c > 0$ transitions as the function of $1/N$. Boxes correspond to the $A \rightarrow 2A$, $2A \rightarrow \emptyset$, while circles to the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model. The line shows a fitting of the form (10)

The cluster mean-field method applied for nonequilibrium models first by [18,19] are based on the calculation of N -block probabilities of the model. This method has successfully predicted the phase diagram of many systems. I apply it for one dimensional, site restricted lattice versions of the models mentioned before. It is well known that such approximations predict the phase structure qualitatively well in 1d. It provides an efficient phase diagram exploration method and could give valid results in higher dimensions too (see example [13]). One can set up a master equations for the P_N block probabilities as

$$\frac{\partial P_N(\{s_i\})}{\partial t} = f(P_N(\{s_i\})) , \quad (5)$$

where the site variables take the values: $s_i = \emptyset, A$. During the solution of these equations one estimates larger than N sized block probabilities by the maximum overlap approximation like

$$P_{N+1}(s_1, \dots, s_{N+1}) \simeq \frac{P_N(s_1, \dots, s_N)P_N(s_2, \dots, s_{N+1})}{P_N(s_2, \dots, s_N, \emptyset) + P_N(s_2, \dots, s_N, A)} . \quad (6)$$

Taking into account spatial symmetries, for the maximal $N = 8$ approximations of this work one has to find the solution of equations of 136 independent variables. Using this method first I investigated the model defined by the transition probabilities

$$A \xrightarrow{\sigma} 2A, \quad 2A \xrightarrow{\lambda} \emptyset, \quad \emptyset A \xrightarrow{D} A\emptyset . \quad (7)$$

The steady state solutions have been determined for $N = 1, 2, 3, \dots, 8$ approximations and the corresponding steady state densities $\rho_s(\sigma, D)$ are calculated numerically. The phase transition points are obtained for several values and are plotted in the σ_c/D vs. λ_c/D parameterization on plot (Fig.1(a)) in order to be comparable with the results of [16]. The phase transition lines for $N > 1$ corroborate the phase diagram of [16], with $(\lambda_c/D)_{th} > 0$ threshold values and with linear shapes in the $\sigma/D \rightarrow \infty$ limit. By inspecting the numerical values of the $(\lambda_c/D)_{th}(N)$ thresholds values for $N = 2, 3, \dots, 8$ (see Table I) one can setup a hypothesis that in general

$$(\lambda_c/D)_{th}(N) = 2/(N-1) \quad (8)$$

exactly. Therefore one can extrapolate that in the $N \rightarrow \infty$ limit $(\lambda_c/D)_{th}(N) \rightarrow 0$ (Fig.1(b)) in agreement with the results of [16] for 1d. So $N > 1$ cluster mean-field approximations, which can take into account the diffusion exhibit similar phase diagram as the one obtained by the NPRG method and in the asymptotic limit they even reproduce the zero threshold corresponding to 1d.

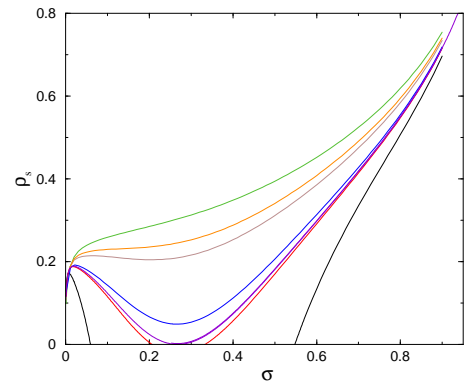


FIG. 2. Steady state density results in the $N = 7$ approximations of the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model. Different curves correspond to: $D = 1, 0.7, 0.6, 0.4, 0.371, 0.36, 0.2$ (top-to bottom). The $\sigma_c > 0$ critical point disappears for $D^* > 0.37083$.

The other system of interest in this study is the

$$A \xrightarrow{\sigma} 2A, \quad 4A \xrightarrow{\lambda} \emptyset, \quad \emptyset A \xrightarrow{D} A\emptyset \quad (9)$$

model, for which perturbative RG predicts $d_c = 2/3$ [17], therefore in all physical dimensions only type (4) mean-field transitions are expected at $\sigma_c = 0$. By solving the

cluster mean-field equations up to $N = 8$, with $\lambda = 1 - \sigma$ parameterization one obtains a reentrant phase structure for low diffusion rates as in case of the $2A \rightarrow 3A$, $4A \rightarrow \emptyset$ model [12] (Fig.2). I have determined the $(\lambda_c/D)_{th}$ threshold values for each N and plotted them as the function of $1/N$ (Fig.1(b)). One can see a tendency towards level-off contrary to the results for the $A \rightarrow 2A$, $2A \rightarrow \emptyset$ case. By extrapolating to the $N \rightarrow \infty$ limit using a form similar, but more general than (8)

$$(\lambda_c/D)_{th}(N) = a + b/(N - 1)^c \quad (10)$$

the threshold does not vanishes : $a = 1.2$, $b = 34.5$, $c = 2.14$, therefore we may expect phase transitions with $\sigma_c > 0$ even in one dimension for any $0 < D \leq 1$ diffusion probabilities.

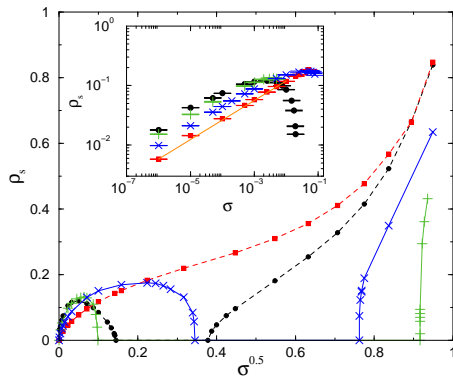


FIG. 3. Simulation results for the steady state density of the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model. Crosses correspond to $D = 1.0$, “+” signs to $D = 0.2$ diffusions in 1d. Circles denote $D = 0.01$, squares $D = 1$ data in 2d. Error bars are smaller than the symbol sizes. The lines serve to guide the eye. The insert shows the data magnified in the neighborhood of the $\sigma = 0$ transition point. The solid line shows a power-law fitting with the exponent $\beta = 0.33(1)$.

To test the cluster mean-field results for the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model I performed simulations in one dimension with lattice sizes: $L = 10^5$ and with periodic boundary conditions. The simulations were started from homogeneously filled lattices with probability $1/2$. One elementary Monte Carlo step consist of the following sub-steps. A particle and a direction are selected randomly. A particle hopping is attempted in the given direction with probability D provided the nearest neighbour (nn) site was empty. If the diffusion attempt was unsuccessful either 4 nn particles in the given direction are removed with probability λ or an offspring is created in an empty nn site in the direction selected before. The time (t) measured by Monte Carlo steps (MCS) is updated by $\Delta t = 1/n$, where n is the total number of particles. The density of particles $\rho(t)$ is followed up to 10^7 MCS (throughout the whole paper the time is measured by Monte Carlo steps (MCS)).

The phase transition points have been located for several diffusion rates and are shown on Fig.3. A qualitative agreement with the low- D results of the finite N -cluster mean-field approximations can be observed. However the $\sigma_c > 0$ transition persists even for $D = 1$ diffusion probability in agreement with the $N \rightarrow \infty$ extrapolations.

The density decay near a $\sigma_c > 0$ critical point, at $D = 0.2$ has been investigated in more detail. The density at σ_c is expected to decay as (3). Fig.4(a) shows the local slopes of α defined as

$$\alpha_{eff}(t) = \frac{-\ln[\rho(t)/\rho(t/m)]}{\ln(m)}, \quad (11)$$

(where I used $m = 2$). As one can see curves with $\sigma > 0.8398$ veer up (active phase), while those with $\sigma < 0.8398$ veer down (absorbing phase). A clean scaling with $\alpha = 0.159(1)$ exponent can be observed at $\sigma = 0.83980(2)$ corroborating the 1+1 dimensional DP class exponent value ($\alpha = 0.159464(6)$ [20]). In the inactive phase $\rho(t)$ vanishes exponentially in agreement with the DP behavior again. One may expect the same kind of transition all along the $\sigma_c(D) > 0$ transition line. Indeed simulations showed that the density decays in a similar way at transition points with $D = 0.01, 0.05, 0.09$.

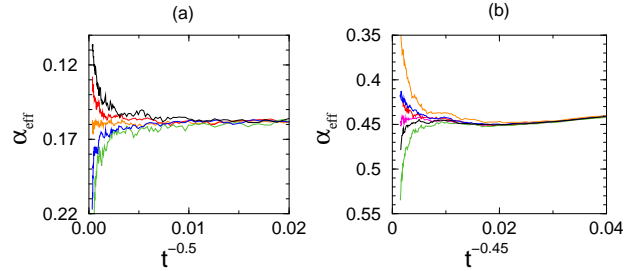


FIG. 4. (a) Local slopes of the density decay exponent α as the function of $t^{-0.5}$ of the the one-dimensional $A \rightarrow 2A$, $4A \rightarrow \emptyset$ model at $D = 0.2$. Different curves correspond to $\sigma = 0.8399, 0.83985, 0.8398, 0.83975, 0.8397$ (top to bottom). The critical point is located at $\sigma_c = 0.83980(2)$. (b) The same as in (a) in two dimensions, for $\sigma = 0.1426, 0.14262, 0.14263, 0.14264, 0.14265, 0.1427$ (top to bottom).

The simulations for this model were repeated in two dimensions in $L = 4 \times 10^3$ linear sized systems with periodic boundary conditions. These simulations were started from fully occupied lattices. One elementary Monte Carlo step consists of the following processes. A particle and a number $x_1 \in (0, 1)$ are selected randomly; if $x_1 < D$ a site exchange is attempted with one of the randomly selected nn. The time is updated by $1/n$. A particle and a number $x_2 \in (0, 1)$ are selected randomly. If $x_2 < \sigma$ and if the number of nn empty sites is greater than 0, one new particle is created at an empty site selected randomly. If $x_2 \geq \sigma$ and the number of nn particles is greater than 2, four randomly selected neighboring particles are removed. The time (t) is updated by

$1/n$ again. The density of particles was followed up to $t_{max} \leq 10^7$ MCS. As one can see simulation data (Fig.3) and the 7-point approximations (Fig.2) fit qualitatively well (this is true for other $N > 1$ levels as well). In both cases for weak diffusion rates reentrant phase transitions occur with $\sigma_c > 0$, while for strong diffusions only a single phase transition at $\sigma_c = 0$ branching rate can be found. The density decay at $D = 0.01$ is analyzed near the phase transition point. The local slope figure shows a separatrix for the critical value $\sigma_c = 0.14263(1)$ as can be seen on Fig.4(b). One can read-off the corresponding decay exponent $\alpha = 0.445(5)$, which agrees with the 2+1 dimensional DP value ($\alpha = 0.4505(10)$ [21]).

I also investigated the steady state behavior at the $\sigma_c = 0$ transition. The steady state density in the active phase near the critical phase transition point is expected to scale as eq.(2). As the insert of Fig.3 shows by applying power-law fitting in the $10^{-6} \leq \sigma \leq 10^{-3}$ region one obtains $\beta \simeq 0.33(1)$ both in one and two dimensions at different diffusion rates. This agrees with the mean-field value (4) for this model. The density at $\sigma_c = 0$ decays as $\rho \propto t^{-1/3}$ trivially, dictated by the $4A \rightarrow \emptyset$ process.

In conclusion numerical evidence is provided that the $A \rightarrow 2A$, $4A \rightarrow \emptyset$ branching and annihilating random walk process exhibits diffusion dependent phase transitions contrary the expectations coming from perturbative renormalization. In particular N -cluster mean-field approximations (with extrapolations to the $N \rightarrow \infty$ limit) resulted in a reentrant (D - σ) phase diagram, with phase transitions at $\sigma_c > 0$ for $0 < D \leq 1$ diffusion probabilities. Simulations have shown that along this transition line DP critical behavior occurs in one and two dimensions. This type of critical behavior is the consequence of an effective $A \rightarrow \emptyset$ reaction generated by $A \rightarrow 2A \rightarrow 3A \rightarrow 4A \rightarrow \emptyset$ of slowly moving particles. In one dimension this line of phase transitions persist for all $0 < D \leq 1$ diffusions, while in 2d it disappears for high diffusion rates. For any D and d values a mean-field transition, characterized by $\beta = 1/3$ occurs at $\sigma_c = 0$.

Similar reentrant phase diagram has been observed in case of the one dimensional $A \rightarrow 2A$, $3A \rightarrow \emptyset$ model [22], in a variant of the NEKIM model [23] and in the $2A \rightarrow 3A$, $4A \rightarrow \emptyset$ model [12,13]. In all cases the diffusion competes with particle reaction processes, and the bare parameters should somehow form renormalized reaction rates which govern the evolution over long times and distances. An other study using exact methods [24] showed that the particle density fluctuations undergo a diffusion dependent phase transition in the bosonic PCPD model for $d > 2$. A very recent, non-perturbative RG study [16] has found similar diffusion dependent phase diagram in the $A \rightarrow 2A$, $2A \rightarrow \emptyset$ model. That work points out that non-perturbative effects arise and there is a threshold $(\lambda_c/D)_{th}(d)$ above which DP, while below it a type (4) mean-field transition at $\sigma_c = 0$ appears. The present N -cluster approximations confirm those results and even-

tuate similar phase diagram as in [16] for any finite N , with a threshold value: $(\lambda_c/D)_{th}(N) = 2/(N - 1)$. In the $N \rightarrow \infty$ limit this corroborates a vanishing threshold in 1d [16].

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- [1] J. Marro and R. Dickman, *Nonequilibrium phase transitions in lattice models*, Cambridge University Press, Cambridge, 1999.
 - [2] H. Berry, Phys. Rev. E **67**, 031907 (2003).
 - [3] J.-P. Bouchaud, A. Georges, Phys. Rep. **195**, 127 (1990).
 - [4] H. Hinrichsen, Adv. Phys. **49**, 815 (2000)
 - [5] U. Täuber, Adv. in Solid State Phys. **43** 659 (2003).
 - [6] G. Ódor, Rev. Mod. Phys. **76** (2004) in press, eprint: cond-mat/0205644.
 - [7] G. Ódor and N. Menyhárd, Physica D **168**, 305 (2002).
 - [8] I. Jensen and R. Dickman, Phys. Rev. E **48**, 1710 (1993); I. Jensen, Phys. Rev. Lett. **70**, 1465 (1993).
 - [9] H. Hinrichsen and G. Ódor, Phys. Rev. E **58**, 311 (1998).
 - [10] G. Ódor, Phys. Rev. E **67**, 056114 (2003).
 - [11] K. Park, H. Hinrichsen and I. Kim, Phys. Rev. E **66**, 025101 (2002).
 - [12] G. Ódor, Phys. Rev. E **69**, 036112 (2004).
 - [13] G. Ódor, cond-mat/0403562.
 - [14] Confirmed by H. Chaté in a private communication.
 - [15] L. Canet, B. Delamotte, O. Deloubrière and N. Wschebor, Phys. Rev. Lett. **92**, 195703 (2004).
 - [16] L. Canet, H. Chaté and B. Delamotte, cond-mat/0403423.
 - [17] J. L. Cardy and U. C. Täuber, J. Stat. Phys. **90**, 1 (1998).
 - [18] H. A. Gutowitz, J. D. Victor and B. W. Knight, Physica **28D**, 18, (1987).
 - [19] R. Dickman, Phys. Rev. A **38**, 2588, (1988).
 - [20] I. Jensen, J. Phys. A **32**, 5233 (1999).
 - [21] C. A. Voigt and R. M. Ziff, Phys. Rev. E **56**, R6241 (1997).
 - [22] R. Dickman, Phys. Rev. B **40**, 7005 (1989); R. Dickman, Phys. Rev. A **42**, 6985 (1990).
 - [23] N. Menyhárd and G. Ódor, Phys. Rev. E **68**, (2003) 056106.
 - [24] M. Paessens, G. M. Schuetz, J. Phys. A **37** (2004) 4709.

N	2	3	4	5	6	7	8
$(\lambda_c/D)_{th}$	2	1	0.666	0.5	0.4	0.333	0.286

TABLE I. Numerical N -cluster results for the threshold values of the $A \rightarrow 2A$, $2A \rightarrow \emptyset$ model